

supplementary materials

Acta Cryst. (2014). E70, o481 [doi:10.1107/S1600536814006187]

5-Cyclopentyl-2-methyl-3-(3-methylphenylsulfonyl)-1-benzofuran

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1. Comment

As a part of our ongoing study of 5-cyclopentyl-2-methyl-1-benzofuran derivatives containing phenylsulfonyl (Seo *et al.*, 2011) and 4-bromophenylsulfonyl (Choi *et al.*, 2012) substituents in the 3-position, we report here on the crystal structure of the title compound.

In the title molecule (Fig. 1), the benzofuran ring system is essentially planar, with a mean deviation of 0.015 (2) Å from the least-squares plane defined by the nine constituent atoms. The 3-methylphenyl ring is essentially planar, with a mean deviation of 0.008 (2) Å from the least-squares plane defined by the six constituent atoms. The cyclopentyl ring has an envelope conformation. The dihedral angle formed by the benzofuran ring system and the 3-methylphenyl ring is 78.44 (8)°.

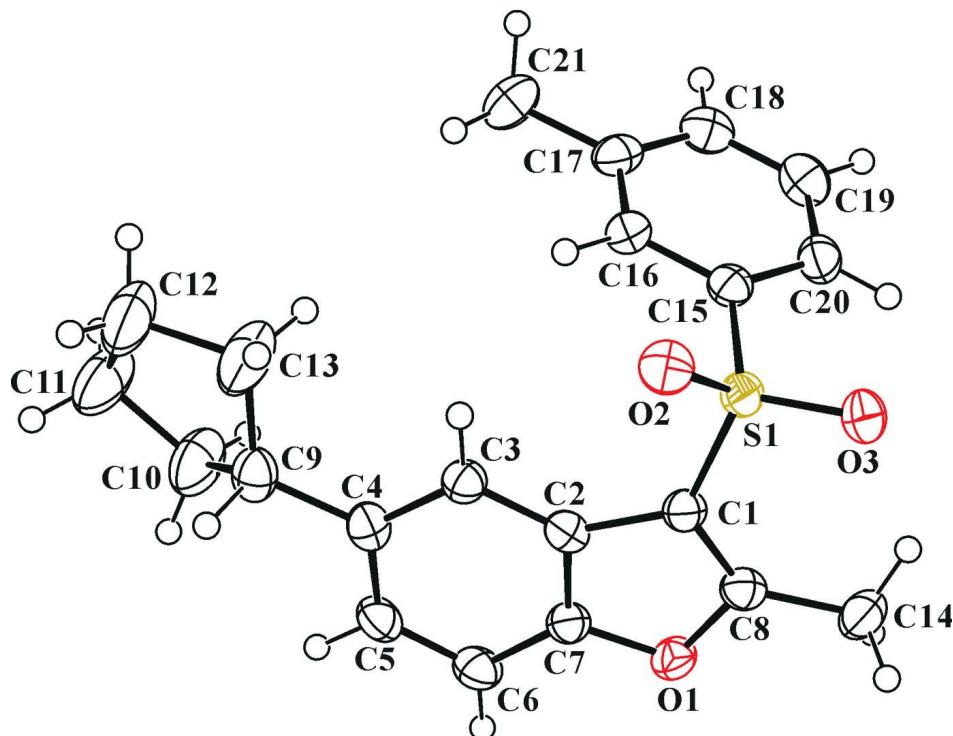
In the crystal structure (Fig. 2), the molecules are linked by C—H···O hydrogen bonds (Table 1) related by gliding plane a perpendicular to *b*-axis. The chains of C—H···O bonded molecules are stacked by C—H···π interactions (Table 1, Cg1 is the centroid of the C15–C20 3-methylphenyl-ring), resulting in a two-dimensional supramolecular layers.

2. Experimental

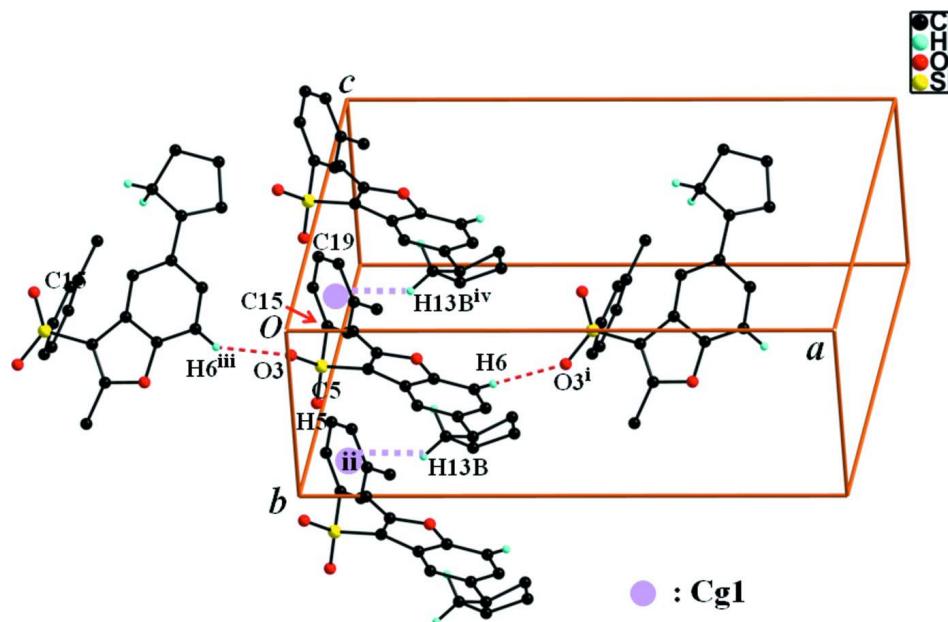
3-Chloroperoxybenzoic acid (77%, 448 mg, 2.0 mmol) was added in small portions to a stirred solution of 5-cyclopentyl-2-methyl-3-(3-methylphenylsulfanyl)-1-benzofuran (290 mg, 0.9 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 10 h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (benzene) to afford the title compound as a colorless solid [yield 73%, m.p. 417–418 K; $R_f = 0.48$ (benzene)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in acetone at room temperature.

3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aryl, 1.00 Å for methine, 0.99 Å for methylene and 0.98 Å for methyl H atoms, respectively. U_{iso} (H) = 1.2 U_{eq} (C) for aryl, methine and methylene, and 1.5 U_{eq} (C) for methyl H atoms. The positions of methyl hydrogens were optimized using the SHELXL-97's command AFIX 137 (Sheldrick, 2008).

**Figure 1**

The molecular structure of the title molecule with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. The hydrogen atoms are presented as small spheres of arbitrary radius.

**Figure 2**

A view of the C—H···O and C—H···π interactions (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $x + 1/2, -y + 1/2, z$; (ii) $x, y + 1, z$; (iii) $x - 1/2, -y + 1/2, z$; (iv) $x, y - 1, z$.]

